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The Hausdorff moments in statistical mechanics

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A new method for solving the Hausdorff moment problem is presented which makes use of Pollaczek polynomials. This problem is severely ill posed; a regularized solution is obtained without any use of prior knowledge. When the problem is treated in the L^2 space and the moments are finite in number and affected by noise or round-off errors, the approximation converges asymptotically in the L^2 norm. The method is applied to various questions of statistical mechanics and in particular to the determination of the density of states. Concerning this latter problem the method is extended to include distribution valued densities. Computing the Laplace transform of the expansion a new series representation of the partition function $Z(\beta)$ ($\beta=1/k_BT$) is obtained which coincides with a Watson resummation of the high-temperature series for $Z(\beta)$.

I. INTRODUCTION

The classical Hausdorff moment problem can be formulated as follows:
Problem: Given a sequence of real numbers $\{\mu_k\}_0^\infty$ find a function u such that

$$\int_0^1 x^k u(x)dx=\mu_k \quad (k=0,1,2,...). \tag{1}$$

The Hausdorff moment problem occurs in several questions of statistical mechanics such as the determination of the frequency spectrum in a harmonic solid or the radial distribution in a polymer chain. Moreover the partition function is the Laplace transform of the density of states, and if this latter has compact support, then it is possible to expand the partition function in a power series whose coefficients can be written in terms of the moments μ_k. In many problems of physical interest the density of states cannot be expressed in terms of a function u, but requires the introduction of distributions.

The Hausdorff moment problem is ill posed in the sense of Hadamard.[1] In order to make clear this point we introduce a solution space X and a data space Y. Suppose that $X=L^2(0,1)$; then Eq. (1) can be rewritten as a scalar product in L^2: i.e., $(u,x^k)_{L^2(0,1)}=\mu_k$ and $Y=l^2$. Now the operator $A:L^2(0,1)\to l^2$, defined by Eq. (1) is continuous, but its inverse A^{-1} is not continuous, because the range of A is only dense in l^2. Therefore the solution of the Hausdorff moment problem is unique but it does not depend continuously on the data. Furthermore, in practical cases, we have at our disposal only a finite number of moments $\{\mu_k\}_0^N$; therefore we must look for the solution not in the space X, but in a linear finite-dimensional subspace of X, i.e., X_{N+1}. Now any function which is orthogonal to X_{N+1} cannot be recovered. We can say that the components of u orthogonal to X_{N+1} are the invisible ones. In such a case the solution is not unique. Nevertheless we have in this case a continuous dependence of the solution on the data and this is due to the fact that the problem is dealt with in finite-dimensional spaces. Continuous dependence of the solution on the data, however, does not yield numerical stability. In fact the problem of determining the component of u onto X_{N+1} can be reduced to the inversion of matrices and this last problem can be ill conditioned when the smallest eigenvalues

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cluster near zero, while the others spread elsewhere. It is possible to evaluate the condition number[2] for the finite Hausdorff moment problem and one finds that it increases very rapidly as N increases; this fact explains the large instabilities which can be observed in the numerical treatment of the finite Hausdorff moment problem.

No mathematical trickery can remedy the lack of information. But there are several methods which can treat the data in such a way that numerical instabilities are avoided and a *regularized solution* is obtained. The method which has received, up to now, greater attention in the mathematical literature is the so-called Tikhonov's method.[1] When applied to the finite Hausdorff moment problem it consists in minimizing a functional which can be obtained by combining Eq. (1) with a constraint derived by some *a priori* information on the solution. Another procedure, which is popular among physicists, is the so-called maximum-entropy method. It consists in maximizing the entropy functional[3,4] and it gives a sequence of weakly convergent approximations. However, since results on more stringent forms of convergence are not available, the discussions concerning this method are essentially based on "extensive empirical evidence".[4] The maximum-entropy method has been applied to various problems of statistical physics, molecular physics, and solid state physics (the relevant literature can be traced from Ref. 4).

Here we present and apply to various problems of statistical mechanics a new regularized method for the solution of the classical Hausdorff moment problem. The mathematical foundation of this method has already been discussed and proven by one of us in Ref. 5. In the present article we focus our attention on the applications of the method to various questions of statistical mechanics and we extend it to include distribution-valued densities of states. The most significant advantages of our method are the following:

(1) it does not require any *a priori* information on the solution;

(2) if the data (the Hausdorff moments) are noiseless and infinite in number, the solution is represented by a series expansion converging in the sense of L^2 norm;

(3) if the data are finite in number (let us say $N+1$) and affected by noise (e.g., the round-off errors in the numerical determination of the moments), the series above (see point 2) diverges, but it still converges asymptotically, in the sense of L^2, as $N\to\infty$ and $\epsilon\to 0$ (ϵ being a bound of the noise);

(4) the method can be extended to include distribution-valued densities of states;

(5) we can perform the Laplace transform of the series which represents the density of states, obtaining an expansion of the partition function with good properties of convergence;

(6) the method is efficient and fast from a numerical viewpoint.

As a disadvantage we note that the method cannot include, in a natural way, the *a priori* information on the positivity of the density of states.

The article is organized as follows: in Sec. II we introduce the method and we obtain the representation of the partition function through the Laplace transform. In Sec. III all the numerical questions connected with the fact that the moments are finite in number and affected by errors are discussed in detail and illustrated through numerical examples. Section IV is devoted to the applications to statistical mechanics. In Appendix A we present the Watson resummation of the high-temperature series of the partition function. In Appendix B we consider the extension of the method to distribution-valued densities. Finally in Appendix C we give the recursion formulas necessary to implement the algorithm.

II. SOLUTION OF THE HAUSDORFF MOMENT PROBLEM

A. Solution by the use of Pollaczek functions

Let us suppose, for the moment, that the function $u(x)$, in Eq. (1), belongs to $L^2(0,1)$. Hausdorff[6] has given necessary and sufficient conditions for the sequence $\{\mu_k\}_0^\infty$ to be the moments of a function u belonging to $L^2(0,1)$. Furthermore Riesz[7] proved that in such a case the following inequality holds true:

$$\sum_{k=0}^{\infty} |\mu_k|^2 < \pi \int_0^1 |u(x)|^2 dx \tag{2}$$

and π cannot be replaced by any smaller constant. Then, at first, we suppose that the sequence $\{\mu_k\}_0^\infty$ is a moment sequence which satisfies the Hausdorff conditions and the inequality (2).

Let us put $x=\exp(-t)$ in Eq. (1); then we obtain

$$\mu_k = \int_0^\infty \exp[-(k+1/2)t]\exp(-t/2)u[\exp(-t)]dt. \tag{3}$$

Therefore the moments μ_k may be regarded as the values, at the points $z=(k+1/2)$, of the Laplace transform $\tilde{f}(z)$ of the function $f(t)$ defined as follows:

$$f(t) = \begin{cases} \exp(-t/2)u[\exp(-t)], & \text{for } t \geqslant 0 \\ 0, & \text{for } t<0, \end{cases} \tag{4}$$

where $t=\log(1/x)$. We have $\mu_k=\tilde{f}(k+1/2)$. Furthermore, since we have assumed that $u \in L^2(0,1)$, then from the Plancherel Theorem it follows that also $\tilde{f}(iy) \in L^2(-\infty,+\infty)$; in fact we have

$$\int_{-\infty}^{+\infty} |f(t)|^2 dt = \int_0^1 |u(x)|^2 dx = \frac{1}{2\pi} \int_{-\infty}^{+\infty} |\tilde{f}(iy)|^2 dy. \tag{5}$$

Moreover from Eq. (2) it follows that

$$\sum_{k=0}^{\infty} |\mu_k|^2 < \frac{1}{2} \int_{-\infty}^{+\infty} |\tilde{f}(iy)|^2 dy. \tag{6}$$

Now let us introduce the Pollaczek polynomials. They are a set of polynomials $P_n^\lambda(y)$, orthogonal in $(-\infty,+\infty)$ with the weight function[8]

$$w(y) = \frac{1}{\pi} 2^{(2\lambda-1)} |\Gamma(\lambda+iy)|^2,$$

where $\lambda>0$. Hereafter we shall take $\lambda=1/2$, and this index will be omitted. Then the orthonormality condition reads

$$\int_{-\infty}^{+\infty} w(y)P_m(y)P_n(y)dy = \delta_{n,m}, \tag{7}$$

where now $w(y) = |\Gamma(iy+1/2)|^2/\pi$. These polynomials can be easily evaluated by the use of the recurrence relation given in Appendix C. Next we introduce the following functions (called hereafter Pollaczek functions):

$$\psi_n(y) = \frac{1}{\sqrt{\pi}} \Gamma(\tfrac{1}{2}+iy)P_n(y); \quad (P_0(y)=1), \tag{8}$$

which form a complete basis in $L^2(-\infty,+\infty)$.[9]

Since $\tilde{f}(iy) \in L^2(-\infty,+\infty)$, then we can expand $\tilde{f}(iy)$ as

$$\tilde{f}(iy) = \sum_{n=0}^{\infty} c_n \psi_n(y). \tag{9}$$

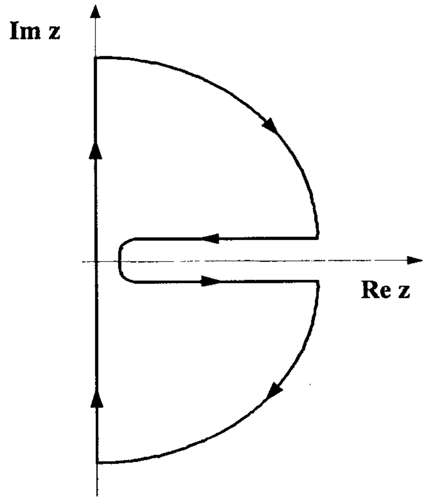

FIG. 1. Integration path for the evaluation of the integral of Eq. (10).

From the orthogonality property [Eq. (7)] it follows that

$$c_n = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \tilde{f}(iy)\Gamma(\tfrac{1}{2}-iy)P_n(y)dy. \tag{10}$$

The right-hand side (rhs) of Eq. (10) can be evaluated by the contour method; indeed taking an integration path as shown in Fig. 1 we obtain

$$\begin{cases} c_n = 2\sqrt{\pi} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \tilde{f}(k+\tfrac{1}{2})P_n[-i(k+\tfrac{1}{2})] \\ \tilde{f}(k+\tfrac{1}{2}) = \mu_k \quad (k=0,1,2,...,). \end{cases} \tag{11}$$

Therefore from the moment sequence $\{\mu_k\}_0^\infty$ we recover uniquely the function $\tilde{f}(iy)$ and the convergence of the expansion (9) is in the sense of the L^2 norm.

Now denoting the Fourier-transform operator by $\mathscr{F}$ ($\mathscr{F}^{-1}$ is the inverse Fourier transform operator), we have

$$f(t) = \mathscr{F}^{-1}\{\tilde{f}(iy)\} = \sum_{n=0}^{\infty} c_n \mathscr{F}^{-1}\{\psi_n(y)\}. \tag{12}$$

Since

$$\Gamma(\tfrac{1}{2}+iy) = \int_0^{+\infty} \exp(-s)s^{(iy-1/2)}\, ds \tag{13}$$

putting $s=\exp(-t)$, we get

$$\Gamma(\tfrac{1}{2}+iy) = \int_{-\infty}^{+\infty} \exp(-iyt)\exp[-\exp(-t)]\exp(-t/2)dt. \tag{14}$$

Then we have

$$\mathscr{F}^{-1}\{\psi_0(y)\}=\frac{1}{\sqrt{\pi}}\exp(-t/2)\exp[-\exp(-t)] \tag{15}$$

and moreover

$$\mathscr{F}^{-1}\{\psi_n(y)\}=P_n\left(-i\frac{d}{dt}\right)\left\{\frac{1}{\sqrt{\pi}}\exp(-t/2)\exp[-\exp(-t)]\right\}. \tag{16}$$

Finally, returning to the variable $x=\exp(-t)$, we obtain

$$u(x)=\sum_{n=0}^{\infty}c_n\frac{1}{\sqrt{\pi x}}\left\{P_n\left(ix\frac{d}{dx}\right)\sqrt{x}\exp(-x)\right\}=\frac{1}{\sqrt{2\pi}}\sum_{n=0}^{\infty}c_n\Phi_n(x)=\sum_{n=0}^{\infty}u_n\Phi_n(x), \tag{17}$$

where $u_n=c_n/\sqrt{2\pi}$ and the functions $\Phi_n(x)$ are given by

$$\begin{cases}\Phi_n(x)=B_n(x)\exp(-x)\\ B_n(x)=i^n\sqrt{2}L_n(2x),\end{cases} \tag{18}$$

$L_n(x)$ being the Laguerre polynomials. The functions $\Phi_n(x)$ form a complete basis in $L^2(0,+\infty)$.[5]

B. Representation of the partition function

Equation (17) gives a series representation of the density of states $u(x)$, assuming that $u\in L^2(0,1)$ and where x has the physical meaning of an energy. The series (17) converges, in the sense of the L^2 norm, to the function u for $x\in(0,1)$, and it tends to zero (always in the sense of L^2) outside the interval (0,1). In order to obtain a representation of the partition function $Z(\beta)$, $\beta=1/k_BT$ (k_B is the Boltzmann constant, T is the absolute temperature), we perform the Laplace transform of the density $u(x)$, i.e.,

$$Z(\beta)=\int_0^{+\infty}\exp(-\beta x)u(x)dx=\int_0^{+\infty}\exp(-\beta x)\left[\sum_{n=0}^{\infty}u_n\Phi_n(x)\right]dx. \tag{19}$$

Next we exchange the integral with the sum; this exchange is legitimate if $\beta>0$ (see also the next section)

$$Z(\beta)=\sum_{n=0}^{\infty}u_n\int_0^{\infty}\exp[-(\beta+1)x]B_n(x)dx. \tag{20}$$

Finally we evaluate the Laplace transform of the functions $\Phi_n(x)=B_n(x)\exp(-x)$. The polynomials $B_n(x)$ are proportional to the polynomials of Laguerre and the latter can be written as

$$L_n(x)=\sum_{k=0}^{n}\binom{n}{k}\frac{(-x)^k}{k!}. \tag{21}$$

Then we have

$$\int_0^{+\infty}\exp(-sx)L_n(2x)dx=\sum_{k=0}^{n}\binom{n}{k}\frac{2^k}{k!}\frac{d^k}{ds^k}\left(\frac{1}{s}\right)=\sum_{k=0}^{n}\binom{n}{k}(-2)^k s^{-(k+1)}. \tag{22}$$

Putting $s=1+\beta$, and $\beta=\exp\alpha$, we obtain

$$\sum_{k=0}^{n} \binom{n}{k} \frac{(-2)^k}{[1+\exp(\alpha)]^k} = \left(\frac{\exp(\alpha)-1}{\exp(\alpha)+1}\right)^n = \left[\tanh\left(\frac{\alpha}{2}\right)\right]^n. \tag{23}$$

From Eqs. (18), (19), (22), and (23), we have

$$Z(\alpha) = \sum_{n=0}^{\infty} u_n \chi_n(\alpha), \tag{24}$$

where

$$\chi_n(\alpha) = (\sqrt{2})^{-1} \frac{\exp(-\alpha/2)}{\cosh(\alpha/2)} [i \tanh(\alpha/2)]^n. \tag{25}$$

The expansion (24) can also be obtained by a Watson resummation of the high-temperature expansion of the partition function (see Appendix A); the latter reads

$$Z(\beta) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \mu_k \beta^k, \tag{26}$$

μ_k being the Hausdorff moments. The series (26) is slowly convergent for high values of β (i.e., low temperatures); on the contrary the expansion (24) has a satisfactory rate of convergence in the range of medium and low temperatures, and it is slowly convergent for high temperatures. However we can accelerate its convergence rate even at high temperatures with the following trick. We multiply each of the data μ_k by a cutoff factor of the type $1/c^k (c>1)$. Indeed if we perform a Watson resummation (see Appendix A) of the following high-temperature series of the partition function

$$Z(\alpha-\gamma) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \mu_k \exp(-k\gamma) \exp(k\alpha) \equiv Z_\gamma(\alpha) \tag{27}$$

(where $\alpha = \log \beta$, $\gamma = \log c$) we obtain

$$Z_\gamma(\alpha) = \frac{1}{\sqrt{2}} \frac{\exp(-\alpha/2)}{\cosh(\alpha/2)} \sum_{n=0}^{\infty} u_n^{(\gamma)} \{i \tanh(\alpha/2)\}^n. \tag{28}$$

The coefficients $u_n^{(\gamma)}$ are given by

$$u_n^{(\gamma)} = \frac{1}{\sqrt{2}} \sum_{n=0}^{\infty} \frac{(-1)^k}{k!} \mu_k \exp(-k\gamma) P_n[-i(k+1/2)]. \tag{29}$$

Now we observe that $Z(\alpha) \equiv Z_\gamma(\alpha+\gamma)$, that is,

$$Z(\alpha) = \frac{1}{\sqrt{2}} \frac{\exp[-(\alpha+\gamma)/2]}{\cosh[(\alpha+\gamma)/2]} \sum_{n=0}^{\infty} u_n^{(\gamma)} \{i \tanh[(\alpha+\gamma)/2]\}^n; \tag{30}$$

therefore with this simple trick we can compute the value of the partition function at α by evaluating Z_γ in $\alpha+\gamma$: in a region where the convergence rate is better. The rate of convergence of this approximation of the partition function is as good as the Euler resummation of the high-temperature series.

III. NUMERICAL ANALYSIS

Up to now we have supposed that the moments μ_k are both infinite in number and noiseless. But we know that in practice we can evaluate only a finite number of them and moreover they are necessarily affected by a round-off numerical error. In such a situation one cannot hope that the series (17) converges in the sense of the L^2 norm. Indeed it diverges; but we can still prove that it converges, in the sense of the L^2 norm, asymptotically as the number of the moments (the data) tends to infinity and the noise goes to zero.

Let us focus our attention on the expansion (17). We denote by $c_n^{(\epsilon,N)}$ (or accordingly by $u_n^{(\epsilon,N)}$) the coefficients of this expansion when the data are finite in number [i.e., we know only $(N+1)$ moments] and they are perturbed by noise. We denote by $\mu_k^{(\epsilon)}$ the Hausdorff moments affected by a numerical error ϵ, i.e., $|\mu_k^{(\epsilon)}-\mu_k|\leqslant\epsilon$. Then we can write

$$c_n^{(\epsilon,N)}=2\sqrt{\pi}\sum_{k=0}^{N}\frac{(-1)^k}{k!}\mu_k^{(\epsilon)}P_n[-i(k+\tfrac{1}{2})] \tag{31}$$

and accordingly $u_n^{(\epsilon,N)}=c_n^{(\epsilon,N)}/\sqrt{2\pi}$. The following statements hold true:

(i) $\Sigma_{n=0}^{\infty}|u_n^{(0,\infty)}|^2=\|u\|^2_{L^2(0,1)}=C$ where C is a constant;

(ii) $\Sigma_{n=0}^{\infty}|u_n^{(\epsilon,N)}|^2=+\infty$;

(iii) $\lim_{\substack{N\to\infty\\ \epsilon\to 0}} u_n^{(\epsilon,N)}=u_n^{(0,\infty)}$, $\forall n$, where we must firstly take the limit for $N\to\infty$;

(iv) if $n_0(\epsilon,N)$ is defined as

$$n_0=\max\left\{m\in\mathbf{N}:\sum_{n=0}^{m}|u_n^{(\epsilon,N)}|^2<C\right\}$$

then

$$\lim_{\substack{N\to\infty\\ \epsilon\to 0}} n_0(\epsilon,N)=+\infty \tag{32}$$

(for the proof of these statements see Ref. 5).

Remark: In (ii) the relation remains true even if $\epsilon=0$. Moreover let us remind that if $N\to\infty$, but $\epsilon>0$, the moments do not satisfy the Hausdorff condition; in particular Carlsonian interpolation (see Appendix A and Ref. 10) no longer works.

Next we can write the approximation of the density of states

$$u^{(\epsilon,N)}(x)=\sum_{n=0}^{n_0(\epsilon,N)}u_n^{(\epsilon,N)}\Phi_n(x) \tag{33}$$

and we have the following:

Proposition 1: *The equality*

$$\lim_{\substack{N\to\infty\\ \epsilon\to 0}}\|u-u^{(\epsilon,N)}\|_{L^2(0,+\infty)}=0 \tag{34}$$

holds true (for the proof see Ref. 5).

At this point we must solve the problem of the numerical determination of the truncation point $n_0(\epsilon,N)$. Let us recall that the coefficients $u_n^{(\epsilon,N)}$ are given by

$$u_n^{(\epsilon,N)}=\sum_{k=0}^{N}d_k^{(\epsilon)}P_n[-i(k+\tfrac{1}{2})], \tag{35}$$

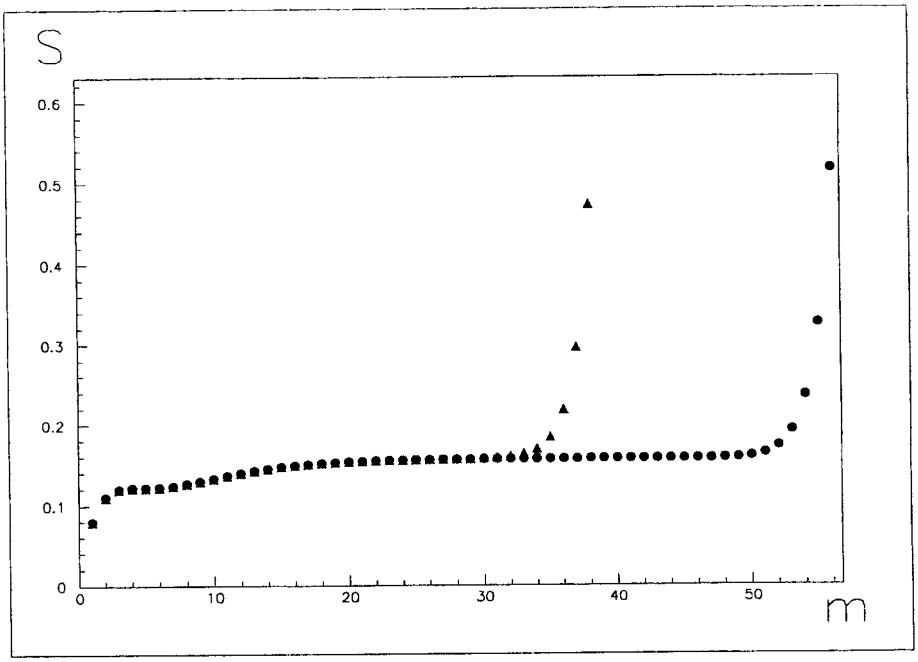

FIG. 2. The sum $S=\Sigma_{n=0}^{m}|u_n^{(\epsilon,N)}|^2$ is plotted vs m for $N=15$ (filled triangles) and for $N=20$ (filled circles); $\epsilon=10^{-6}$. The coefficients $u_n^{(\epsilon,N)}$ have been computed for the function: $u(x)=10x\exp(-10x)$, if $0\leqslant x\leqslant 1$, 0, otherwise.

where $d_k^{(\epsilon)}=\sqrt{2}(-1)^k\mu_k^{(\epsilon)}/k!$. Furthermore the asymptotic behavior of the Pollaczek polynomials for large values of n is given by[5]

$$P_n[-i(k+\tfrac{1}{2})]\sim\frac{(-1)^n i^n}{k!}(2n)^k. \tag{36}$$

Then for n sufficiently large we have that

$$\lim_{n\to\infty}\frac{\Sigma_{k=0}^{(N-1)}|d_k^{(\epsilon)}P_n[-i(k+1/2)]|}{|d_N^{(\epsilon)}P_n[-i(N+1/2)]|}=0 \tag{37}$$

and therefore it follows that, for n sufficiently large, $|u_n^{(\epsilon,N)}|\geqslant|d_N^{(\epsilon)}P_n[-i(N+1/2)]|$. It follows that the terms $|u_n^{(\epsilon,N)}|$, for n sufficiently large, increase at least as $(n)^N$. Now we can plot the sum $\Sigma_{n=0}^{m}|u_n^{(\epsilon,N)}|^2$ vs m. If ϵ is sufficiently small and N sufficiently large, this sum shows a plateau, corresponding to that value of m such that $\Sigma_{n=0}^{m}|u_n^{(\epsilon,N)}|^2$ attains the value $C=\|u\|^2_{L^2(0,1)}$ (or at least a value very close to C). Successively this sum increases very fast, because any term $|u_n^{(\epsilon,N)}|$ increases, as a function of n, at least as $(n)^N$. Therefore it is very easy to determine, from a numerical viewpoint, the maximum integer such that $\Sigma_{n=0}^{m}|u_n^{(\epsilon,N)}|^2\leqslant C$, which is precisely $n_0(\epsilon,N)$. A numerical example is presented in Fig. 2 and the corresponding reconstruction is shown in Fig. 3. In this example we have taken ϵ very small, i.e., of the order of magnitude of the numerical round-off error.

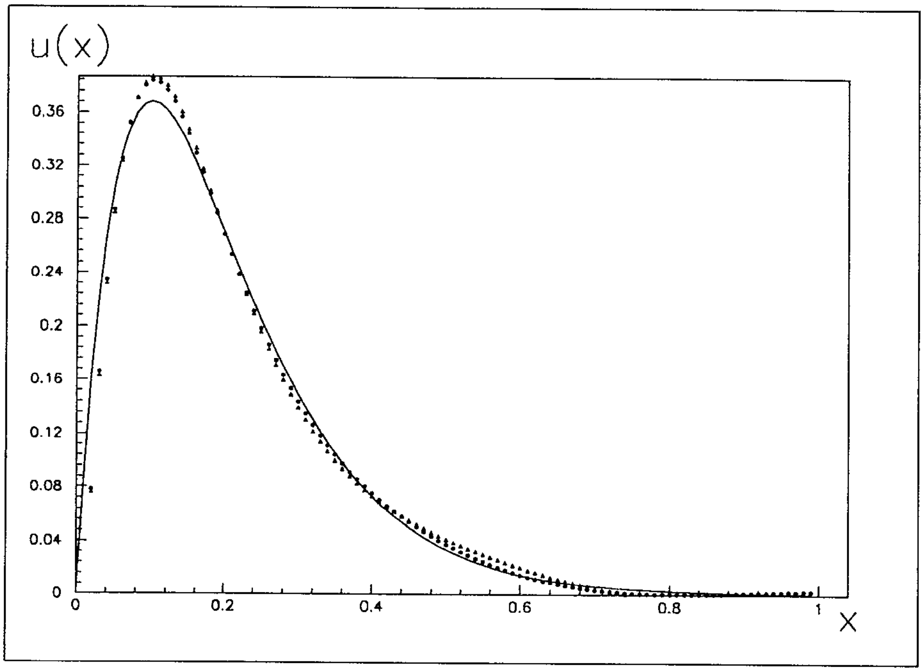

FIG. 3. Reconstruction of the function $u(x)$ of Fig. 2 both for $N=15$, $n_0=30$ (filled triangles) and for $N=20$, $n_0=45$ (filled circles).

Concerning the series representation of the partition function [Eq. (24)], we can proceed as follows. We rewrite the expansion (24) in this way

$$Z(\beta)=\frac{\sqrt{2}}{(\beta+1)}\sum_{n=0}^{\infty}u_n^{(0,\infty)}i^n\left(\frac{\beta-1}{\beta+1}\right)^n; \quad [\beta=\exp(\alpha)] \tag{38}$$

and accordingly we have the following approximation:

$$Z^{(\epsilon,N)}(\beta)=\frac{\sqrt{2}}{(\beta+1)}\sum_{n=0}^{n_0(\epsilon,N)}u_n^{(\epsilon,N)}i^n\left(\frac{\beta-1}{\beta+1}\right)^n. \tag{39}$$

Next we can prove the following Proposition.

Proposition 2: *The following equality holds true:*

$$\lim_{\substack{N\to\infty\\ \epsilon\to 0}}|Z(\beta)-Z^{(\epsilon,N)}(\beta)|=0, \quad (\beta>0). \tag{40}$$

Proof: We can write

$$|Z(\beta)-Z^{(\epsilon,N)}(\beta)|=\frac{\sqrt{2}}{\beta+1}\left\{\left|\sum_{n=0}^{n_0(\epsilon,N)}[(\beta-1)/(\beta+1)]^n(u_n^{(0,\infty)}-u_n^{(\epsilon,N)})\right.\right.$$

$$\left.\left.+\sum_{n=n_0(\epsilon,N)+1}^{\infty}[(\beta-1)/(\beta+1)]^n u_n^{(0,\infty)}\right|\right\}$$

$$\leqslant\frac{\sqrt{2}}{\beta+1}\left\{\left|\sum_{n=0}^{n_0(\epsilon,N)}[(\beta-1)/(\beta+1)]^n(u_n^{(0,\infty)}-u_n^{(\epsilon,N)})\right|\right.$$

$$\left.+\left|\sum_{n=n_0(\epsilon,N)+1}^{\infty}[(\beta-1)/(\beta+1)]^n u_n^{(0,\infty)}\right|\right\}. \tag{41}$$

Now, using the Schwarz inequality, we get from the first term on the rhs of Eq. (41)

$$\left|\sum_{n=0}^{n_0(\epsilon,N)}[(\beta-1)/(\beta+1)]^n(u_n^{(0,\infty)}-u_n^{(\epsilon,N)})\right|$$

$$\leqslant\left(\sum_{n=0}^{n_0(\epsilon,N)}|(\beta-1)/(\beta+1)|^{2n}\right)^{1/2}\left(\sum_{n=0}^{n_0(\epsilon,N)}|u_n^{(0,\infty)}-u_n^{(\epsilon,N)}|^2\right)^{1/2}. \tag{42}$$

Now for $N\to\infty$ and $\epsilon\to 0$, the second factor on the rhs of Eq. (42) tends to zero [see Proposition 1 and Ref. 5 Eq. (52)], while the first factor converges to a finite value if $\beta>0$. Analogously we obtain

$$\left|\sum_{n=n_0(\epsilon,N)+1}^{\infty}[(\beta-1)/(\beta+1)]^n u_n^{(0,\infty)}\right|$$

$$\leqslant\left(\sum_{n=n_0(\epsilon,N)+1}^{\infty}|(\beta-1)/(\beta+1)|^{2n}\right)^{1/2}\left(\sum_{n=n_0(\epsilon,N)+1}^{\infty}|u_n^{(0,\infty)}|^2\right)^{1/2}. \tag{43}$$

Since both the first and the second factor are the remainders of a convergent series if $\beta>0$, then in view of formula (32), the limit for $\epsilon\to 0$ and $N\to\infty$ of the rhs of Eq. (43) is zero and the proposition is proved.

IV. APPLICATIONS TO STATISTICAL MECHANICS

In this section we shall consider three examples taken from different branches of statistical mechanics.

A. Radial distribution in polymer physics

The first example concerns the radial distribution in polymer physics. To this purpose let us consider the distribution $W(\mathbf{r})$ of the vector distance $\mathbf{r}$ between the first and the last skeletal atoms of a polymer chain.[11,12] Then $W(\mathbf{r})d\mathbf{r}$ is the probability that the last atom of the chain is situated within a volume element $d\mathbf{r}$ located at $\mathbf{r}$ relative to the first atom. If the system is rotationally invariant, then W depends only on the magnitude of $\mathbf{r}$, which we denote by r. In the limit of very long polymers, unperturbed by self-interactions of long range and by external constraints, W is a Gaussian distribution. We remind the reader that the main self-interaction of long range is the so-called excluded volume effect. However, for finite chains, W is no longer Gaussian. If the distribution function is known, the moments can of course be evaluated from

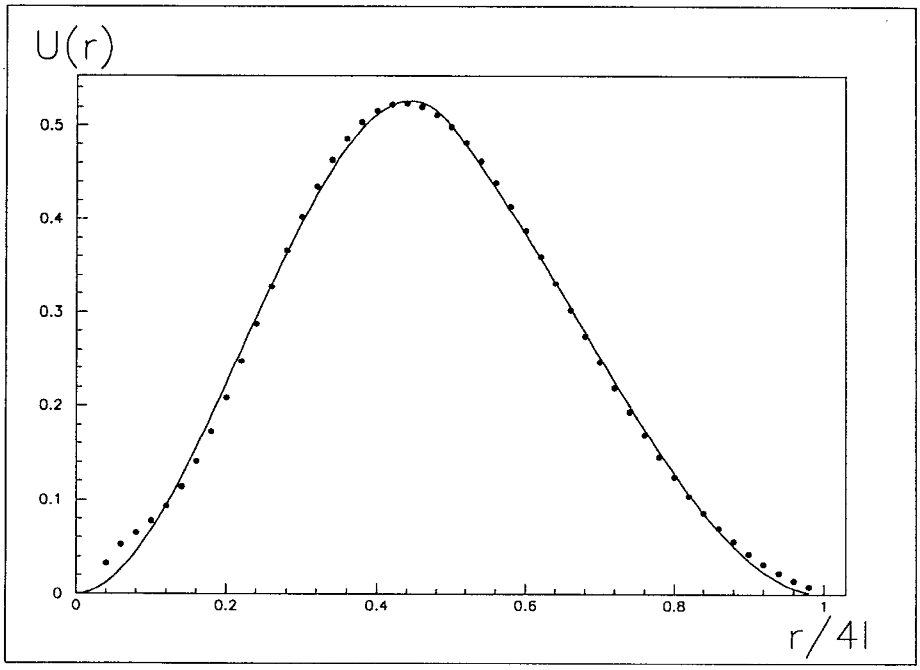

FIG. 4. Reconstruction of the radial distribution function $U(r)=4\pi r^2 W_4(r)$ vs $r/4l$. The solid line is the exact function, the dots represent the approximation obtained with $N=25$, $n_0=30$.

it. If not, moments of the distribution often can be evaluated independently without recourse to the distribution function which usually is less readily susceptible to determination.[11]

For purposes of illustration we consider an exactly solved problem: the so-called freely jointed chain, a polymer with the lengths of the bonds fixed, the bond angles unconstrained, and without excluded volume. This problem has been partially solved by Rayleigh.[13] Treloar[14] found the exact expansion for the distribution $W_m(r)$ of a chain of $m+1$ skeletal atoms

$$W_m(r)=(8\pi r l^2)^{-1} m(m-1) \sum_{t=0}^{\tau} \frac{(-1)^t}{t!(m-t)!} \left\{\frac{m-(r/l)-2t}{2}\right\}^{m-2}, \tag{44}$$

where τ is specified by the following inequality:

$$\left\{\frac{m-(r/l)}{2}\right\}-1 \leqslant \tau \leqslant \left\{\frac{m-(r/l)}{2}\right\}, \tag{45}$$

l being the bond length. $W_m(r)$ vanishes for $r>ml$.

We have tested our method by reconstructing the radial distribution function $4\pi r^2 W_4(r)$; in Fig. 4 we plot this function versus $r/4l$. The dots represent the reconstruction obtained from Eq. (33) using 26 moments; the truncation index is $n_0=30$. The moments used in the approximation have been evaluated from Eq. (44) with $m=4$.

B. Frequency spectrum in harmonic crystals

As a second example we try the derivation of the frequency spectrum in harmonic three-dimensional crystals. This calculation can be reduced to the diagonalization of a matrix.[15] The analytical diagonalization is usually impossible and numerical diagonalization techniques are

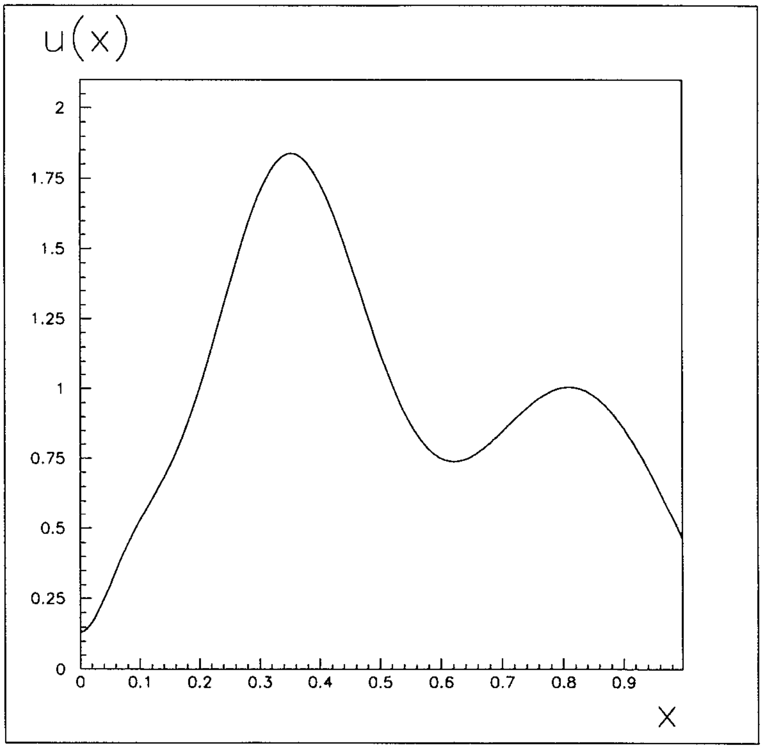

FIG. 5. Frequency density $u(x)$ for the FCC crystal obtained with $N=30$, $n_0=75$.

cumbersome and sometimes cannot be implemented with sufficient accuracy.[4] On the contrary the moment method can provide valuable substitutes for exact solutions.[16–18]

We want to recover the frequency spectrum $g(\omega)$ from the knowledge of its moments; g is a function of compact support, and when the maximum frequency ω_0 is known, it can be rescaled so that it vanishes for $\omega>1$. Usually it is possible to compute the even moments of $g(\omega)$ (Refs. 16–19)

$$\mu_k=\int_0^1 \omega^{2k} g(\omega)d\omega, \tag{46}$$

which involve the computation of traces rather than eigenvalues of a given matrix. The moment problem (46) can be reduced to its standard form by introducing a new density through the substitutions

$$\begin{cases} x=\omega^2, \\ g(\omega)d\omega=u(x)dx, \\ g(\omega)=2\omega u(\omega^2). \end{cases} \tag{47}$$

Then Eq. (46) reads

$$\mu_k=\int_0^1 x^k u(x)dx. \tag{48}$$

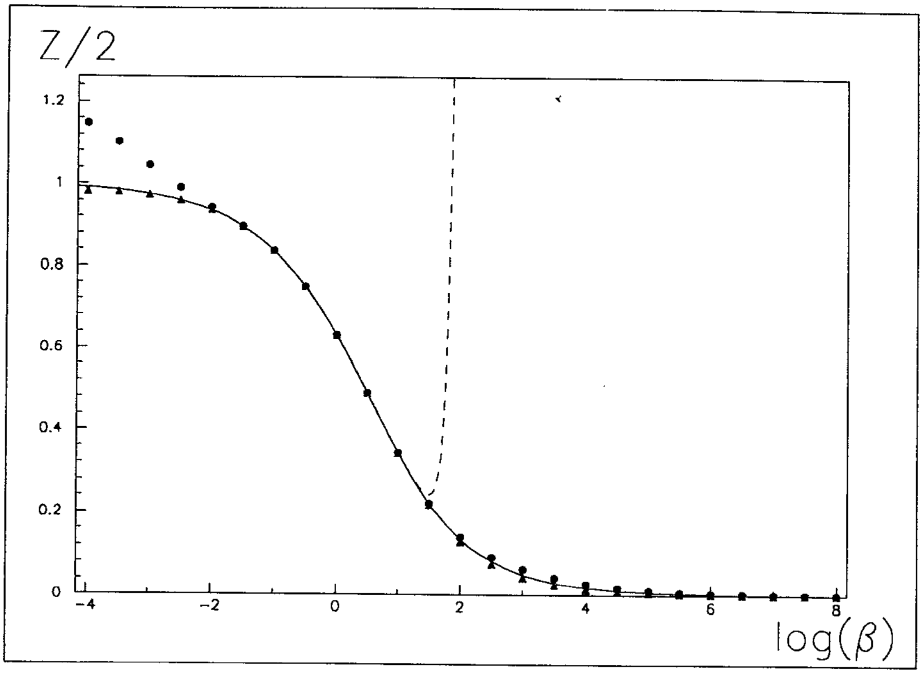

FIG. 6. Partition function $Z/2$ vs $\log \beta$ for the model described in the text. Solid line: exact partition function; dashed line: Kramers series with $N=10$; filled circles: approximation with $N=10$, $n_0=12$; filled triangles: approximation with a cutoff $c=2.3$ ($N=10$, $n_0=12$).

If the density of states were known, various thermodynamic quantities could be computed such as the internal energy and the specific heat. The zero-temperature limit of the internal energy, which is given by

$$E_0=\frac{1}{2}\int_0^1 \sqrt{x}u(x)dx, \tag{49}$$

deserves particular interest. Isenberg[19] developed a method to compute a large number of moments and applied it to the face centered cubic (FCC) crystal. He evaluated 35 moments. In Fig. 5 we present a reconstruction of $u(x)$ obtained by the use of 31 moments ($N=30$) and truncating the approximation at $n_0=75$. The result is consistent with the known Van Hove singularities[20] located at $x=1/4$, $x=1/2$, and $x=(2+\sqrt{2})/4$. In these points the function $u(x)$ has singular derivatives. We find for E_0 [Eq. (49)] the value $E_0=0.335\,416\,1$, which is not far from the upper and lower bounds evaluated by Wheeler and Gordon[21,22] (i.e., $0.340\,880\,7<E_0<0.340\,888\,3$).

Our numerical method, as well as that based on maximum entropy,[4] is not able to separate the singularities located at $x=1/4$ and $x=1/2$. They produce a single bump centered at $x\sim0.35$. This effect is quite natural in an inverse ill-posed problem. We can say that in our procedure the incorporation of higher moments is well controlled through the L^2-norm convergence, while the maximum-entropy method seems not yet capable of handling a large number of moments.[4] In spite of these advantages our approximation does reproduce in a less satisfactory way than the maximum-entropy method[4] the cusp located at $x=(2+\sqrt{2})/4=0.853$.

C. The partition function

As a third example we evaluate the partition function of a classical particle in a V-shaped potential well

$$V(x)=\begin{cases} |x|, & \text{for} \quad |x|\leqslant 1 \\ \infty, & \text{for} \quad |x|>1. \end{cases} \tag{50}$$

In this case the density of states $u(x)$ is a constant function, and the moments μ_k are given by

$$\mu_k=\frac{2}{k+1}. \tag{51}$$

The canonical partition function reads

$$Z(\beta)=\frac{2[1-\exp(-\beta)]}{\beta}. \tag{52}$$

In Fig. 6 we plot $Z/2$ vs $\alpha=\log \beta$. The exact function is represented by a solid curve; the filled circles give the approximation of $Z/2$ obtained by the use of Eq. (39) with $N=10$, $n_0=12$. It can be seen that the convergence is better than that obtained by the high-temperature series (represented by the dashed line), for medium and low temperatures, while for high temperatures the convergence is slower. However if we introduce a cutoff c (see the end of Sec. II) we improve the rate of convergence even at high temperatures. This is again shown in Fig. 6 where the triangles correspond to the values obtained with $c=2.3$.

Remark: As a final remark we must honestly point out that our method does not work very well in the presence of discontinuities of $u(x)$. In particular if jump discontinuities are present, typical oscillations of the Gibbs-type arise in the neighborhood of these discontinuities. Indeed, as we stated in the previous section, the convergence of the expansion (33) is only an L^2-norm convergence. Things are better in the approximate computation of the partition function $Z(\beta)$. In fact in this case we have a uniform-norm convergence of the expansion (39) (see Proposition 2).

ACKNOWLEDGMENTS

It is a pleasure to thank our friend Professor A. C. Levi for many useful discussions.

APPENDIX A: WATSON RESUMMATION OF THE HIGH-TEMPERATURE EXPANSION

In this appendix we still assume that $u\in L^2(0,1)$. Next we write the Mellin transform of u, i.e.,

$$\mathscr{U}(s)=\int_0^1 x^{(s-1)}u(x)dx. \tag{A1}$$

From a Paley–Wiener-type theorem for the Mellin transform we can prove that

(i) $\mathscr{U}(s)$ is a holomorphic function in the half plane $\{s:\text{Re}(s)>1/2\}$.

(ii) $\int_{-\infty}^{+\infty}|\mathscr{U}(x+iy)|^2\,dy$ is bounded by a constant independent of x, as $1/2<x<\infty$.

(iii) From the Plancherel theorem for the Mellin transform it follows that

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty}|\mathscr{U}(1/2+iy)|^2\,dy=\int_0^1|u(x)|^2\,dx<\infty. \tag{A2}$$

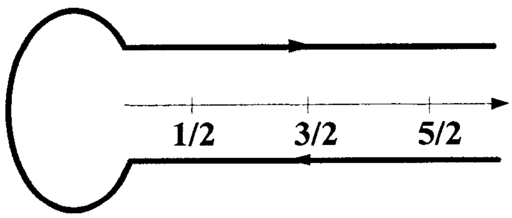

FIG. 7. Integration path C for Eq. (A5).

Moreover the moments $\{\mu_k\}_0^\infty$ can be regarded as the restriction of $\mathscr{U}(s)$ to the positive integers. Therefore in view of the properties (i), (ii), (iii), and of the Carlson theorem,[10] which can be applied in the present case, we can interpolate in a unique way the moments $\{\mu_k\}_0^\infty$ by an interpolating function $\mu(s)=\mathscr{U}(s+1)$. The properties (i), (ii), (iii) above can be restated for the function $\mu(s)$ with a shift of -1 of the half plane $\mathrm{Re}(s)>1/2$.

Now let us recall the expression of the high-temperature expansion

$$Z(\beta)=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\mu_k\beta^k, \quad \beta=1/k_BT. \tag{A3}$$

We rewrite the expansion (A3) as follows:

$$Z(\alpha)=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\mu_k\exp(k\alpha) \quad (\alpha=\log\beta). \tag{A4}$$

Now we can apply the Watson summation method to the expansion (A4). Indeed the terms $(-1)^k/k!$ are the residues of the Euler gamma function $\Gamma(1/2-s)$ at the points $s=k+1/2$. Assuming, for the moment, that $\mathrm{Im}\,\alpha=0, |\mathrm{Re}\,\alpha|<\pi$, in order to guarantee, via the Carlson theorem,[10] the uniqueness of the interpolation, we obtain

$$Z(\alpha)=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\mu_k\exp(k\alpha)=\frac{1}{2\pi i}\int_C\Gamma(1/2-s)\mu(s-1/2)\exp[\alpha(s-1/2)]ds, \tag{A5}$$

where C is a counterclockwise path encircling the positive real semiaxis of the complex s plane (see Fig. 7). Now we may close the contour C, adding two quarters of a circle in the first and in the fourth quadrant and closing the path along the imaginary axis of the s plane. From the Cauchy theorem it follows that

$$\oint_\gamma\Gamma(1/2-s)\mu(s-1/2)\exp[\alpha(s-1/2)]ds=0, \tag{A6}$$

where γ is the closed path indicated in Fig. 1. Furthermore the contribution of the two quarters of a circle, in the first and in the fourth quadrant, vanish (and this follows from the asymptotic behavior of the integrand). Finally we obtain

$$\int_C \Gamma(1/2-s)\mu(s-1/2)\exp[\alpha(s-1/2)]ds$$

$$=i\int_{-\infty}^{+\infty} \Gamma(1/2-iy)\mu(iy-1/2)\exp[\alpha(iy-1/2)]dy. \tag{A7}$$

Since $\mu(iy-1/2)\in L^2(-\infty,+\infty)$ [see statement (iii), and recall the shift of -1 of the half plane $\mathrm{Re}(s)>1/2$] we can expand this function in terms of Pollaczek functions obtaining

$$\mu(iy-1/2)=\sum_{n=0}^{\infty} c_n\psi_n(y). \tag{A8}$$

Then from formulas (A6), (A7), and (A8) it follows that

$$Z(\alpha)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} \Gamma(1/2-iy)\mu(iy-1/2)\exp[\alpha(iy-1/2)]dy$$

$$=\frac{\exp(-\alpha/2)}{2\pi\sqrt{\pi}}\sum_{n=0}^{\infty} c_n\int_{-\infty}^{+\infty} \Gamma(1/2-iy)\Gamma(1/2+iy)P_n(y)\exp(i\alpha y)dy, \tag{A9}$$

where the coefficients c_n are given by Eq. (11). Since $\Gamma(1/2-iy)\Gamma(1/2+iy)=\pi/\cosh(\pi y)$, we have

$$\int_{-\infty}^{+\infty} \frac{P_n(y)}{\cosh(\pi y)}\exp(i\alpha y)dy=P_n\left(-i\frac{d}{d\alpha}\right)\left\{\frac{1}{\cosh(\alpha/2)}\right\}. \tag{A10}$$

Substituting Eq. (A10) in Eq. (A9) we obtain

$$Z(\alpha)=\frac{\exp(-\alpha/2)}{2\sqrt{\pi}}\sum_{n=0}^{\infty} c_nP_n\left(-i\frac{d}{d\alpha}\right)\left\{\frac{1}{\cosh(\alpha/2)}\right\}=\frac{\exp(-\alpha/2)}{2\sqrt{\pi}\cosh(\alpha/2)}\sum_{n=0}^{\infty} c_n\{i\tanh(\alpha/2)\}^n, \tag{A11}$$

which coincides with the expansion given by Eq. (24). Indeed, for the uniqueness of analytic continuation, we can extend the domain of convergence of the expansion given by Eq. (A11) from the initial domain (i.e., $\mathrm{Im}\,\alpha=0$, $|\mathrm{Re}\,\alpha|<\pi$) to the real axis $-\infty<\mathrm{Re}\,\alpha<+\infty$, corresponding to $\beta>0$.

APPENDIX B: EXTENSION TO DISTRIBUTION-VALUED DENSITIES

Let us consider the following moment formula:

$$\mu_k=\int_0^{\infty} x^k\,d\lambda(x). \tag{B1}$$

If $\lambda(x)$ is a constant for $x>1$, then one obtains Hausdorff moments, which can be regarded as generalized Hausdorff moments if the derivative $d\lambda/dx$ is distribution valued. Hereafter we shall focus our attention on the latter case. To be more specific let us suppose that

$$\lambda(x)=\sum_m a_m\theta(x-x_m), \tag{B2}$$

where θ is the Heaviside function and Σ_m is a finite sum. Now let us put, as in Sec. II, $x=\exp(-t)$, then we can formally write

$$\mu_k = \int_0^{+\infty} \exp(-kt) \left\{ \sum_m a_m \delta(t-t_m) \right\} dt = \sum_m a_m x_m^k, \tag{B3}$$

where $x_m = \exp(-t_m)$. For our convenience (see below) we shall rewrite Eq. (B3) in a slightly different form

$$\mu_k = \int_0^{+\infty} \exp(-kt) \left\{ \exp(t/2) \sum_m a_m \exp(t_m/2) \delta(t-t_m) \right\} \exp(-t) dt. \tag{B4}$$

Indeed we want to reconstruct the "density" $\Sigma_m a_m \exp(t_m/2)\delta(t-t_m)$ from the knowledge of the data μ_k. To this purpose let us introduce the following function:

$$\mu(z) = \sum_m a_m x_m^z = \sum_m a_m \exp(z \log x_m) = \sum_m a_m \exp(-zt_m). \tag{B5}$$

The value of $\mu(z)$ at $z = -1/2 + iy$ is given by

$$\mu(-1/2+iy) = \sum_m a_m \exp(t_m/2) \exp(-iyt_m). \tag{B6}$$

Following the line of Sec. II, as a first task we would like to reconstruct the function $\mu(-1/2+iy)$ starting from the data μ_k. But this function does not belong to $L^2(-\infty,+\infty)$, and therefore the method presented in Sec. II cannot work here. Nevertheless we can multiply each one of the data μ_k by the factor $1/(1+k)$ and accordingly the function $\mu(-1/2+iy)$ will be multiplied by $1/(1/2+iy)$. We obtain the auxiliary function

$$\mu_*(-1/2+iy) = \left[\sum_m a_m \exp(t_m/2) \exp(-iyt_m) \right] \Big/ (1/2+iy), \tag{B7}$$

which belongs to $L^2(-\infty,+\infty)$. Therefore it can be reconstructed with the method of Sec. II, obtaining

$$\mu_*(-1/2+iy) = \sum_{n=0}^{\infty} c_n^* \psi_n(y), \tag{B8}$$

where the coefficients c_n^* are given by

$$c_n^* = 2\sqrt{\pi} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \mu_k \frac{1}{1+k} P_n[-i(k+\tfrac{1}{2})]. \tag{B9}$$

If we take into account that the number of data is finite and they are possibly affected by numerical error, then instead of Eq. (B8), we have the following one:

$$\mu_*^{(\epsilon,N)}(-1/2+iy) = \sum_{n=0}^{n_0(\epsilon,N)} c_n^{*(\epsilon,N)} \psi_n(y), \tag{B10}$$

where $n_0(\epsilon,N)$ and the coefficients $c_n^{*(\epsilon,N)}$ have been defined and introduced in Sec. III. Now we can multiply $\mu_*(-1/2+iy)$ by $(1/2+iy)$ and then apply the inverse Fourier transform. Indeed the following proposition can be proven.

Proposition B1: *The following equality holds true:*

$$\left\langle \sum_m a_m \exp(t_m/2)\delta(t-t_m),\varphi \right\rangle = \lim_{\substack{N\to\infty \\ \epsilon\to 0}} \left\langle \sum_{n=0}^{n_0(\epsilon,N)} c_n^{*(\epsilon,N)} \mathscr{F}^{-1}[(1/2+iy)\psi_n(y)],\varphi \right\rangle, \tag{B11}$$

where φ belongs to the Schwartz space S of test functions and $\langle f,\varphi\rangle$ denotes the Lebesgue integral $\int_{-\infty}^{+\infty} \overline{f(x)}\varphi(x)dx$.

Proof: From the theory of the Fourier transform of tempered distributions and from formula (B6) we have

$$\left\langle \mathscr{F}\left\{ \sum_m a_m \exp(t_m/2)\delta(t-t_m)\right\},\varphi \right\rangle = \left\langle \left\{ \sum_m a_m \exp(t_m/2)\exp(-iyt_m)\right\},\varphi \right\rangle$$

$$=\langle \mu(-1/2+iy),\varphi\rangle. \tag{B12}$$

We can also write

$$\left\langle \left\{ \sum_m a_m \exp(t_m/2)\delta(t-t_m)\right\},\varphi \right\rangle = \langle \mathscr{F}^{-1}[(1/2+iy)\mu_*(-1/2+iy)],\varphi\rangle$$

$$=\tfrac{1}{2}\langle \mathscr{F}^{-1}[\mu_*(-1/2+iy)],\varphi\rangle - \langle \mathscr{F}^{-1}[\mu_*(-1/2+iy)],\varphi'\rangle, \tag{B13}$$

where φ' is the first derivative of φ and it still belongs to S. Taking into account that $\psi_n \in S$, we have similarly

$$\langle \mathscr{F}^{-1}[(1/2+iy)\psi_n(y)],\varphi\rangle = \tfrac{1}{2}\langle \mathscr{F}^{-1}[\psi_n(y)],\varphi\rangle - \langle \mathscr{F}^{-1}[\psi_n(y)],\varphi'\rangle. \tag{B14}$$

Next we can prove that

$$\lim_{\substack{N\to\infty \\ \epsilon\to 0}} \left\{ \left\langle \frac{1}{2} \sum_{n=0}^{n_0(\epsilon,N)} c_n^{*(\epsilon,N)} \mathscr{F}^{-1}[\psi_n(y)],\varphi \right\rangle - \left\langle \sum_{n=0}^{n_0(\epsilon,N)} c_n^{*(\epsilon,N)} \mathscr{F}^{-1}[\psi_n(y)],\varphi' \right\rangle \right\}$$

$$=\tfrac{1}{2}\langle \mathscr{F}^{-1}[\mu_*(-1/2+iy)],\varphi\rangle - \langle \mathscr{F}^{-1}[\mu_*(-1/2+iy)],\varphi'\rangle. \tag{B15}$$

Indeed by the use of the Schwarz inequality we have

$$\int_{-\infty}^{+\infty} \left| \mathscr{F}^{-1}[\mu_*(-1/2+iy)] - \sum_{n=0}^{n_0(\epsilon,N)} c_n^{*(\epsilon,N)} \mathscr{F}^{-1}[\psi_n(y)] |x| \varphi(t) \right| dt$$

$$\leqslant \left(\int_{-\infty}^{+\infty} |\varphi(t)|^2 \right)^{1/2} \times \left(\int_{-\infty}^{+\infty} \left| \mathscr{F}^{-1}[\mu_*(-1/2+iy)] \right.\right.$$

$$\left.\left. - \sum_{n=0}^{n_0(\epsilon,N)} c_n^{*(\epsilon,N)} \mathscr{F}^{-1}[\psi_n(y)] \right|^2 dt \right)^{1/2}. \tag{B16}$$

Recalling formula (12) and Proposition 1, we have that the second term on the rhs of formula (B16) vanishes for $\epsilon \to 0$ and $N \to \infty$, while the first term is finite. The analogous inequality holds true for the difference

$$\int_{-\infty}^{+\infty} \left| \mathscr{F}^{-1}[\mu_*(-1/2+iy)] - \sum_{n=0}^{n_0(\epsilon,N)} c_n^{*(\epsilon,N)} \mathscr{F}^{-1}[\psi_n(y)] |x| \varphi'(t) \right| dt$$

and with similar arguments it can be proven that it also tends to zero for $\epsilon \to 0$, $N \to \infty$. Therefore equality (B15) is proven. Now taking into account the equalities (B13), (B14), and (B15) we can write

$$\lim_{\substack{N\to\infty\\ \epsilon\to 0}} \left\langle \sum_{n=0}^{n_0(\epsilon,N)} c_n^{*(\epsilon,N)} \mathscr{F}^{-1}[(1/2+iy)\psi_n(y)],\varphi \right\rangle$$

$$= \tfrac{1}{2}\langle \mathscr{F}^{-1}[\mu_*(-1/2+iy)],\varphi\rangle - \langle \mathscr{F}^{-1}[\mu_*(-1/2+iy)],\varphi'\rangle$$

$$= \left\langle \left\{ \sum_m a_m \exp(t_m/2)\delta(t-t_m) \right\},\varphi \right\rangle \tag{B17}$$

and this equality proves the Proposition.

Now we can come back to the variable x. In fact we can formally write

$$\sum_m a_m \delta(x-x_m) = \exp(t/2) \sum_m a_m \exp(t_m/2)\delta(t-t_m). \tag{B18}$$

We can easily evaluate the inverse Fourier transform of $\psi_n(y)$ and of $iy\psi_n(y)$ in terms of polynomials $B_n(x)$. Observing that $\exp(t/2) = 1/\sqrt{(x)}$, we finally obtain the formal equality

$$\sum_m a_m \delta(x-x_m) = \lim_{\substack{N\to\infty\\ \epsilon\to 0}} \sum_{n=0}^{n_0(\epsilon,N)} u_n^{*(\epsilon,N)} \exp(-x)\{(x-n)B_n(x) + inB_{n-1}(x)\}, \tag{B19}$$

where $u_n^{*(\epsilon,N)} = c_n^{*(\epsilon,N)}/\sqrt{2\pi}$; the recursion formula of the polynomials $B_n(x)$ is given in the subsequent Appendix C.

APPENDIX C: THE ALGORITHM AND THE RECURSIVE FORMULAS

The algorithm is based on the following formulas:

$$u^{(\epsilon,N)}(x) = \sum_{n=0}^{n_0} u_n^{(\epsilon,N)} \Phi_n(x) \tag{C1}$$

and

$$Z^{(\epsilon,N)}(\beta) = \frac{\sqrt{2}}{(\beta+1)} \sum_{n=0}^{n_0} u_n^{(\epsilon,N)} i^n \left(\frac{\beta-1}{\beta+1}\right)^n; \quad \beta = 1/k_B T, \tag{C2}$$

where

$$\begin{cases} u_n^{(\epsilon,N)} = \sqrt{2} \sum_{k=0}^{N} \frac{(-1)^k}{k!} \mu_k^{(\epsilon)} P_n[-i(k+1/2)], \\ \Phi_n(x) = \exp(-x) B_n(x), \\ B_n(x) = i^n \sqrt{2} L_n(2x). \end{cases} \tag{C3}$$

$P_n(x)$ are the Pollaczek polynomials and $L_n(x)$ are the Laguerre polynomials. The algorithm runs easily if one knows the recursion formulas of the Pollaczek and of the $B_n(x)$ polynomials.

The recurrence relation of the Pollaczek polynomials reads[8]

$$\begin{cases} nP_n(x) - 2xP_{n-1}(x) + (n-1)P_{n-2}(x) = 0 \\ P_{-1} = 0, \quad P_0 = 1, \quad P_1 = 2x. \end{cases} \tag{C4}$$

Concerning the functions $\Phi_n(x)$ they are essentially the inverse Fourier transform of the Pollaczek functions $\psi_n(y)$; indeed we have for $x \geqslant 0$

$$\Phi_n(x) = \sqrt{2\pi/x}\mathscr{F}^{-1}\{\psi_n(y)\} = \sqrt{2/x}\{P_n(ixd/dx)\sqrt{x}\exp(-x)\} = B_n(x)\exp(-x), \tag{C5}$$

where the polynomials $B_n(x)$ satisfy the following recurrence relation:[5]

$$\begin{cases} (n+1)B_{n+1}(x) - i(2n+1-2x)B_n(x) - nB_{n-1}(x) = 0, \\ B_{-1} = 0, \quad B_0 = \sqrt{2}. \end{cases} \tag{C6}$$

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